Property Modelling and Databases in Product-Process Design

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Properties of pure chemicals and their mixtures play an important role in the design of chemical-based products and the processes that manufacture them. Although the use of experimental data in the design and/or analysis of these chemical-based products and their processes is desirable, they are not always available. Also, it may be too expensive or it may take too long to measure the required data. In these situations and when repetitive calculations are involved, as in process simulation, it is useful to have appropriate models to reliably predict the needed properties. For property model development, however, it is necessary to have a large database of measured property data that has been checked for consistency and accuracy. The presentation will first introduce a database, in terms of its knowledge representation structure, the type and range of properties and chemical systems covered, and their internal consistency-accuracy checks. The database includes properties of organic chemicals, polymers and ionic liquids. There are also chemical class specific database sections, such as for solvents, aroma-chemicals, surfactants and emulsifiers. The use of this property database for model development will then be highlighted for a class of predictive models employing the group-contribution^{plus} approach, where, the group-contribution (GC) method is combined with the atom-connectivity index (CI) method. Here, two parallel models are developed using the same dataset. However, during applications for property prediction, only the GC-model is used with the option to estimate missing group-contribution parameters through the CI-model. In this way, the application range of the GC-model is increased without the need for additional experimental data. This procedure for model development and use has been successfully employed for a range of pure component properties, polymer repeat-unit properties as well as mixture properties. For the mixture properties, liquid phase activity coefficients are modelled and then predicted through the UNIFAC-CI method. For bulk-properties of organic chemical mixtures, a GC-CI version of the PC-SAFT is used. The developed database and property prediction models have been combined into a properties-software that allows different product-process design related applications. The presentation will also briefly highlight applications of the software for virtual product-process design applications.